I17

Fast algorithms for hybrid functional electronic structure calculations

Lin Lin
University of California, Berkeley

The Fock exchange operator plays a central role modern quantum chemistry and materials science. Compared to Kohn-Sham density functional theory calculations with local and semi-local exchange-correlation functionals, hybrid functional calculations are significantly more expensive due to the inclusion of a fraction of the Fock operator. The main reason is that the application of the Fock operator is much more costly compared to the application of a semi-local operator. Moreover, hybrid functional calculations can require a larger number of self-consistent field (SCF) iterations. In this talk I will introduce fast algorithms to 1) apply the Fock operator less frequently without losing accuracy 2) reduce the cost of each Fock operator application, and 3) reduce the number of SCF iterations. All these techniques are applicable to insulating as well as metallic systems. We demonstrate that the combination of these techniques can lead to nearly two orders of magnitude speedup for hybrid functional calculations, and can enable hybrid functional calculations in planewave basis sets with more than 4000 atoms. Some of these techniques, such as adaptively compressed exchange formulation (ACE), has already been implemented in community software packages such as Quantum ESPRESSO.